

FORM PTO-1449

## INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO.  
1503.0200006APPLICATION NO.  
09/802,996APPLICANT  
Agrafiotis et al.FILING DATE  
March 12, 2001GROUP  
2123

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## U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AB	AA1	4,773,099	09/1988	Bokser	382	14	
	AB1	4,811,217	03/1989	Tokizane et al.	364	300	
	AC1	4,859,736	08/1989	Rink	525	54.1	
	AD1	4,908,773	03/1990	Pantoliano et al.	364	496	
	AE1	4,935,875	06/1990	Shah et al.	364	497	
	AF1	4,939,666	07/1990	Hardman	364	496	
	AG1	5,010,175	04/1991	Rutter et al.	530	334	
	AH1	5,025,388	06/1991	Cramer, III et al.	364	496	
	AI1	5,155,801	10/1992	Lincoln	395	22	

## FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AB	AJ1	EP 0 355 266 B1	02/1990	EPO	B01J	19/00	Yes No
	AK1	EP 0 355 628 B1	02/1990	EPO	G21F	9/00	No
	AL1	EP 0 770 876 A1	05/1997	EPO	G01N	33/68	Yes No
	AM1	EP 0 818 744 A2	01/1998	EPO	G06F	17/50	Yes No

## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	1	Borg, Ingwer and Groenen, Patrick, <i>Modern Multidimensional Scaling Theory and Applications</i> , Springer Series in Statistics, 1997, entire book submitted.
	AO	1	Agrafiotis, D.K. et al., "Advances in diversity profiling and combinatorial series design," <i>Molecular Diversity</i> , Kluwer Academic Publishers, Vol. 4, 1999, pp. 1-22.
	AP	1	Agrafiotis, D.K. and Lobanov, V.S., "An Efficient Implementation of Distance-Based Diversity Measures Based on <i>k-d</i> Trees," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, Vol. 39, No. 1, January/February 1999, pp. 51-58.
	AQ	1	Agrafiotis, D.K. and Lobanov, V.S., "Bridging The Gap Between Diversity And QSAR," <i>Abstracts of Papers Part 1: 215th ACS National Meeting</i> , March 29-April 2, 1998, p. 181-COMP.
	AR	1	Agrafiotis, D.K. and Jaeger, E.P., "Directed Diversity®: An Operating System For Combinatorial Chemistry," <i>Abstracts of Papers Part 1: 211th ACS National Meeting</i> , March 24-28, 1996, p. 46-COMP.

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Samuel Brooks

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## U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AB	AA2	5,167,009	11/1992	Skeirik	395	27	
	AB2	5,181,259	01/1993	Rorvig	382	36	
	AC2	5,240,680	08/1993	Zuckermann et al.	422	67	
	AD2	5,260,882	11/1993	Blanco et al.	364	499	
	AE2	5,265,030	11/1993	Skolnick et al.	364	496	
	AF2	5,270,170	12/1993	Schatz et al.	435	7.37	
	AG2	5,288,514	02/1994	Ellman	427	2	
	AH2	5,307,287	04/1994	Cramer, III et al.	364	496	
	AI2	5,323,471	06/1994	Hayashi	382	15	

## FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AB	AJ2	WO 91/19735	12/1991	PCT	C07K	7/02	Yes No
	AK2	WO 92/00091	01/1992	PCT	A61K	37/02	Yes No
	AL2	WO 93/20242	10/1993	PCT	C12Q	1/70	Yes No
	AM2	WO 94/28504	12/1994	PCT	G06F	15/60	Yes No

## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	2	Agrafiotis, D.K., "Diversity of Chemical Libraries," <i>Encyclopedia of Computational Chemistry</i> , John Wiley & Sons Ltd, Vol. 1:A-D, 1998, pp. 742-761.
	AO	2	Agrafiotis, D.K., "On the Use of Information Theory for Assessing Molecular Diversity," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, Vol. 37, No. 3, May/June 1997, pp. 576-580.
	AP	2	Agrafiotis, D.K. et al., "Parallel QSAR," <i>Abstracts of Papers Part 1: 217th ACS National Meeting</i> , March 21-25, 1999, p. 50-COMP.
	AQ	2	Agrafiotis, D.K. et al., "PRODEN: A New Program for Calculating Integrated Projected Populations," <i>Journal of Computational Chemistry</i> , John Wiley & Sons, Inc., Vol. 11, No. 9, October 1990, pp. 1101-1110.
	AR	2	Agrafiotis, D.K. and Jaeger, E.P., "Stochastic Algorithms for Exploring Molecular Diversity," <i>Abstracts of Papers Part 1: 213th ACS National Meeting</i> , April 13-17, 1997, p. 16-CINF.

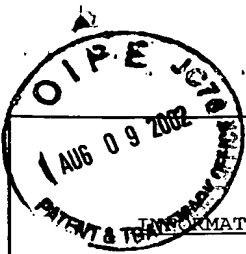
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Samuel B. Bork

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**U.S. PATENT DOCUMENTS**

SIGNATURE DOCUMENTS							
EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AS ↓	AA3	5,331,573	07/1994	Balaji et al.	364	500	Technology Center 2100 AUG 12 2002 RECEIVED
	AB3	5,434,796	07/1995	Weininger	364	496	
	AC3	5,436,850	07/1995	Eisenberg et al.	364	496	
	AD3	5,442,122	08/1995	Noda et al.	564	426	
	AE3	5,463,564	10/1995	Agrafiotis et al.	364	496	
	AF3	5,499,193	03/1996	Sugawara et al.	364	500	
	AG3	5,519,635	05/1996	Miyake et al.	364	497	
	AH3	5,524,065	06/1996	Yagasaki	382	226	
	AI3	5,526,281	06/1996	Chapman et al.	364	496	

**FOREIGN PATENT DOCUMENTS**

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AS ↓	AJ3	WO 95/01606	01/1995	PCT	G06F	15/42	Yes No
	AK3	WO 97/09342	03/1997	PCT	C07H	21/02	Yes No
	AL3	WO 97/20952	06/1997	PCT	C12Q	1/68	Yes No
	AM3	WO 97/27559	07/1997	PCT	G06F	19/00	Yes No

**OTHER (Including Author, Title, Date, Pertinent Pages, etc.)**

AS ↓	AN	3	Agrafiotis, D., "Theoretical Aspects of the Complex: Arts and New Technologies, Applications and Impacts Information Processing '94, North-Holland, Vol. II, 1994, pp. 714-719.
	AO	3	Biswas, G. et al., "Evaluation of Projection Algorithms," <i>IEEE Transactions On Pattern Analysis And Machine Intelligence</i> , IEEE Computer Society, Vol. PAMI-3, No. 6, November 1981, pp. 701-708.
	AP	3	Bonchev, D. and Trinajstić, N., "Information theory, distance matrix, and molecular branching," <i>The Journal of Chemical Physics</i> , American Institute of Physics, Vol. 67, No. 10, November 15, 1977, pp. 4517-4533.
	AQ	3	Chang, C.L. and Lee, R.C.T., "A Heuristic Relaxation Method for Nonlinear Mapping in Cluster Analysis," <i>IEEE Transactions on Systems, Man, and Cybernetics</i> , IEEE Systems, Man, and Cybernetics Society, Vol. SMC-3, March 1973, pp. 197-200.
	AR	3	Cramer, R.D. et al., "Virtual Compound Libraries: A New Approach to Decision Making in Molecular Discovery Research," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, Vol. 38, No. 6, November/December 1998, pp. 1010-1023.

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*Samuel Broda*

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## U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB- CLASS	FILING DATE
MS	AA4	5,545,568	08/1996	Ellman	436	518	
	AB4	5,549,974	08/1996	Holmes	428	403	
	AC4	5,553,225	09/1996	Perry	395	157	
	AD4	5,565,325	10/1996	Blake	435	7.1	
	AE4	5,574,656	11/1996	Agrafiotis et al.	364	500	
	AF4	5,585,277	12/1996	Bowie et al.	436	518	
	AG4	5,602,755	02/1997	Ashe et al.	364	498	
	AH4	5,602,938	02/1997	Akiyama et al.	382	155	
	AI4	5,612,895	03/1997	Balaji et al.	364	496	

## FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB- CLASS	TRANSLATION
MS	AJ4	WO 98/20437	05/1998	PCT	G06F	17/50	Yes No
↓	AK4	WO 98/20459	05/1998	PCT	G06T	11/20	Yes No
	AL4						Yes No
	AM4						Yes No

## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

MS	AN	4	DeMers, D. and Cottrell, G., "Non-Linear Dimensionality Reduction," <i>Advances in Neural Information Processing Systems</i> , Vol. 5, 1993, pp. 580-587.
	AO	4	Frey, P.W. and Slate, D.J., "Letter Recognition Using Holland-Style Adaptive Classifiers," <i>Machine Learning</i> , Kluwer Academic Publishers, Vol. 6, 1991, pp. 161-182.
	AP	4	Friedman, J.H., "Exploratory Projection Pursuit," <i>Journal of the American Statistical Association</i> , American Statistical Association, Vol. 82, No. 397, March 1987, pp. 249-266.
	AQ	4	Friedman, J.H. and Tukey, J.W., "A Projection Pursuit Algorithm for Exploratory Data Analysis," <i>IEEE Transactions on Computers</i> , IEEE Computer Society, Vol. C-23, No. 9, September 1974, pp. 881-889.
	AR	4	Garrido, L. et al., "Use of Multilayer Feedforward Neural Nets As A Display Method for Multidimensional Distributions," <i>International Journal of Neural Systems</i> , World Scientific Publishing Co. Pte. Ltd., Vol. 6, No. 3, September 1995, pp. 273-282.

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## U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AB	AA5	5,634,017	05/1997	Mohanty et al.	395	326	
	AB5	5,635,598	06/1997	Lebl et al.	530	334	
	AC5	5,670,326	09/1997	Beutel	435	7.1	
	AD5	5,679,582	10/1997	Bowie et al.	436	518	
	AE5	5,684,711	11/1997	Agrafiotis et al.	364	500	
	AF5	5,703,792	12/1997	Chapman	364	496	
	AG5	5,712,171	01/1998	Zambias et al.	436	518	
	AH5	5,712,564	01/1998	Hayosh	324	210	
	AI5	5,736,412	04/1998	Zambias et al.	436	518	

## FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ5						Yes No
	AK5						Yes No
	AL5						Yes No
	AM5						Yes No

## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	5	Ghose, A.K. et al., "Prediction of Hydrophobic (Lipophilic) Properties of Small Organic Molecules Using Fragmental Methods: An Analysis of ALOGP and CLOGP Methods," <i>J. Phys. Chem. A</i> , American Chemical Society, Vol. 102, No. 21, May 21, 1998, pp. 3762-3772.
	AO	5	Hall, L.H. and Kier, L.B., "The Molecular Connectivity Chi Indexes and Kappa Shape Indexes in Structure-Property Modeling," <i>Reviews in Computational Chemistry: Advances</i> , VCH Publishers, Inc., 1991, pp. 367-422.
	AP	5	Hecht-Nielsen, R., "Replicator Neural Networks for Universal Optimal Source Coding," <i>Science</i> , American Association for the Advancement of Science, Vol. 269, September 29, 1995, pp. 1860-1863.
	AQ	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," <i>The Journal of Educational Psychology</i> , Warwick and York, Inc., Vol. XXIV, No. 6, September 1933, pp. 417-441.
	AR	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," <i>The Journal of Educational Psychology</i> , Warwick and York, Inc., Vol. XXIV, No. 7, October 1933, pp. 498-520.

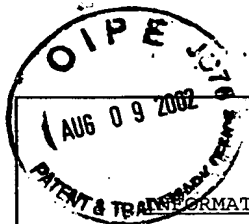
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## U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB- CLASS	FILING DATE
AB	AA6	5,740,326	04/1998	Boulet et al.	395	27	
	AB6	5,789,160	08/1998	Eaton et al.	435	6	
	AC6	5,807,754	09/1998	Zambias et al.	436	518	
	AD6	5,811,241	09/1998	Goodfellow et al.	435	7.1	
	AE6	5,832,494	11/1998	Egger et al.	707	102	
	AF6	5,858,660	01/1999	Eaton et al.	435	6	
	AG6	5,861,532	01/1999	Brown et al.	564	142	
	AH6	5,866,334	02/1999	Beutel	435	6	
	AI6	5,901,069	05/1999	Agrafiotis et al.	364	528.03	

## FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ6						No
	AK6						Yes
	AL6						No
	AM6						Yes
							No

## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	6	Lee, R.C.T. et al., "A Triangulation Method for the Sequential Mapping of Points from N-Space to Two-Space," <i>IEEE Transactions on Computers</i> , The Institute of Electrical and Electronics Engineers, March 1977, pp. 288-292.
	AO	6	Lipinski, C.A. et al., "Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings," <i>Advanced Drug Delivery Reviews</i> , Elsevier Science B.V., Vol. 23, 1997, pp. 3-25.
	AP	6	Lobanov, V.S. and Agrafiotis, D.K., "Intelligent Database Mining Techniques," <i>Abstracts of Papers Part 1: 215th ACS National Meeting</i> , March 29-April 2, 1998, p. 19-COMP.
	AQ	6	Lobanov, V.S. et al., "Rational Selections from Virtual Libraries," <i>Abstracts of Papers Part 1: 217th ACS National Meeting</i> , March 21-25, 1999, p. 181-COMP.
	AR	6	Mao, J. and Jain, A.K., "Artificial Neural Networks for Feature Extraction and Multivariate Data Projection," <i>IEEE transactions on Neural Networks</i> , IEEE Neural Networks, Vol. 6, No. 2, March 1995, pp. 296-317.

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## U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AS		AA7	5,908,960	06/1999	Newlander	564	177
		AB7	5,993,819	11/1999	Haynes et al.	424	188.1
		AC7	6,014,661	01/2000	Ahlberg et al.	707	3
		AD7	6,037,135	03/2000	Kubo et al.	435	7:24
		AE7	6,049,797	04/2000	Guha et al.	707	6
		AF7	6,185,506 B1	02/2001	Cramer et al.	702	19
		AG7					
		AH7					
		AI7					

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	AJ7						Yes No
	AK7						No
	AL7						Yes No
	AM7						Yes No

## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AS	AN	Z	Oja, E., "Principal Components, Minor Components, and Linear Neural Networks," <i>Neural Networks</i> , Pergamon Press Ltd., Vol. 5, 1992, pp. 927-935.
	AO	Z	Patterson, D.E. et al., "Neighborhood Behavior: A Useful Concept for Validation of 'Molecular Diversity' Descriptors," <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 39, No. 16, 1996, pp. 3049-3059.
	AP	Z	Pykett, C.E., "Improving the Efficiency of Sammon's Nonlinear Mapping by Using Clustering Archetypes," <i>Electronics Letters</i> , The Institute of Electrical Engineers, Vol. 14, No. 25, December 7, 1978, pp. 799-800.
	AQ	Z	Rubner, J. and Tavan, P., "A Self-Organizing Network for Principal-Component Analysis," <i>Europhysics Letters</i> , European Physical Society, Vol. 10, No. 7, December 1, 1989, pp. 693-698.
	AR	Z	Sadowski, J. et al., "Assessing Similarity and Diversity of Combinatorial Libraries by Spatial Autocorrelation Functions and Neural Networks," <i>Angewandte Chemie</i> , VCH, Vol. 34, No. 23/24, January 5, 1996, pp. 2674-2677.

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2123**U.S. PATENT DOCUMENTS**

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB- CLASS	FILING DATE
	AA8						
	AB8						
	AC8						
	AD8						
	AE8						
	AF8						
	AG8						
	AH8						
	AI8						

**FOREIGN PATENT DOCUMENTS**

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ8						No
	AK8						No
	AL8						No
	AM8						Yes No

**OTHER (Including Author, Title, Date, Pertinent Pages, etc.)**

MS ↓	AN	8	Thompson, L.A. and Ellman, J.A., "Synthesis and Applications of Small Molecule Libraries," <i>Chemical Reviews</i> , American Chemical Society, Vol. 96, No. 1, January/February 1996, pp. 555-600.
	AO	8	Barnard, John M. and Downs, Geoff M., "Computer representation and manipulation of combinatorial libraries," <i>Perspectives in Drug Discovery and Design</i> , Kluwer Academic Publishers, 1997, pp. 13-30.
	AP	8	Brint, Andrew T. and Willett, Peter, "Upperbound procedures for the identification of similar three-dimensional chemical structures," <i>Journal of Computer-Aided Molecular Design</i> , ESCOM Science Publishers B.V., Vol. 2, No. 4, January 1989, pp. 311-320.
	AQ	8	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 40, No. 15, 1997, pp. 2304-2313.
	AR	8	Gillet, Valerie J. et al., "The Effectiveness of Reactant Pools for Generating Structurally-Diverse Combinatorial Libraries," <i>Journal of Chemical Information Computer Sciences</i> , American Chemical Society, Vol. 37, No. 4, 1997, pp. 731-740.

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*Samuel Breda*

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## PATENT &amp; TRADEMARK INFORMATION DISCLOSURE STATEMENT

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## U.S. PATENT DOCUMENTS

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	AA9						
	AB9						
	AC9						
	AD9						
	AE9						
	AF9						
	AG9						
	AH9						
	AI9						

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## FOREIGN PATENT DOCUMENTS

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	AJ9						Yes No
	AK9						Yes No
	AL9						Yes No
	AM9						Yes No

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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	9	Gillet, Valerie J. et al., "Selecting Combinatorial Libraries to Optimize Diversity and Physical Properties," <i>Journal of Chemical Information Computer Sciences</i> , American Chemical Society, Vol. 39, No. 1, 1999, pp. 169-177.
	AO	9	Kearsley, Simon K. et al., "Chemical Similarity Using Physiochemical Property Descriptors," <i>Journal of Chemical Information Computer Science</i> , American Chemical Society, Vol. 36, No. 1, 1996, pp. 118-127.
	AP	9	Leland, Burton A. et al., "Managing the Combinatorial Explosion," <i>Journal of Chemical Information Computer Science</i> , American Chemical Society, Vol. 37, No. 1, 1997, pp. 62-70.
	AQ	9	Lewis, Richard A. et al., "Similarity Measures for Rational Set Selection and Analysis of Combinatorial Libraries: The Diverse Property-Derived (DPD) Approach," <i>Journal of Chemical Information Computer Science</i> , American Chemical Society, Vol. 37, No. 3, 1997, pp. 599-614.
	AR	9	Martin, Eric J. and Critchlow, Roger E., "Beyond Mere Diversity: Tailoring Combinatorial Libraries for Drug Discovery," <i>Journal of Combinatorial Chemistry</i> , American Chemical Society, Vol. 1, No. 1, 1999, pp. 32-45.

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	AJ10						Yes No
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AB	AN	10	Sheridan, Robert P. et al., "Chemical Similarity Using Geometric Atom Pair Descriptors," <i>Journal of Chemical Information Computer Science</i> , American Chemical Society, Vol. 36, No. 1, 1996, pp. 128-136.
↓	AO	10	Willett, Peter et al., "Chemical Similarity Searching," <i>Journal of Chemical Information Computer Science</i> , American Chemical Society, Vol. 38, No. 6, 1998, pp. 983-996.
↓	AP	10	Agrafiotis, Dimitris K. and Lobanov, Victor S., "Ultrafast Algorithm for Designing Focused Combinational Arrays," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, 2000, Vol. 40, No. 4, pp. 1030-1038.
AB	AQ	10	Ajay et al., "Can We Learn To Distinguish between 'Drug-Like' and 'Nondrug-like' Molecules?" <i>J. Med. Chem.</i> , 1998, American Chemical Society, Vol. 41, No. 18, pp. 3314-3324.
AB	AR	10	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," <i>J. Med. Chem.</i> , American Chemical Society, 1997, Vol. 40, No. 15, pp. 2304-2313.

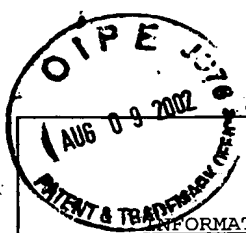
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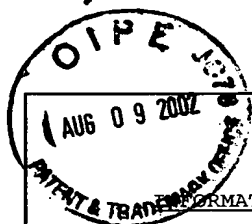
AB	AN	11	Brown, Robert D. and Martin, Yvonne C., "The Information Content of 2D and 3D Structural Descriptors Relevant to Ligand-Receptor Binding," <i>J. Chem. Info. Comput. Sci.</i> , American Chemical Society, 1997, Vol. 37, No. 1, pp. 1-9.
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	AR	11	<i>Daylight Theory: SMARTS</i> (visited September 26, 2000) < <a href="http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html">http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html</a> >, 10 pages.

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	AP	12	Good, Andrew C. and Lewis, Richard A., "New Methodology for Profiling Combinatorial Libraries and Screening Sets: Cleaning Up the Design Process with HARPick," <i>J. Med. Chem.</i> , American Chemical Society, 1997, Vol. 40, No. 24, pp. 3926-3936.
	AQ	12	Gorse, Dominique and Lahana, Roger, "Functional diversity of compound libraries," <i>Current opinion in chemical biology</i> , Elsevier Science Ltd., June 2000, Vol. 4, No. 3, pp. 287-294.
	AR	12	Jamois, Eric A. et al., "Evaluation of Reagent-Based and Product-Based Strategies in the Design of Combinatorial Library Subsets," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, 2000, Vol. 40, No. 1, pp. 63-70.

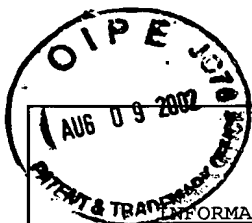
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AB	AN	13	Leach, Andrew R. et al., "Implementation of a System for Reagent Selection and Library Enumeration, Profiling, and Design," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, 1999, Vol. 39, No. 6, pp. 1161-1172.
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AB	AQ	13	Lobanov, Victor S. and Agrafiotis, Dimitris K., "Stochastic Similarity Selections from Large Combinatorial Libraries," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, March/April 2000, Vol. 40, No. 2, pp. 460-470.
↓	AR	13	Matter, Hans and Pötter, Thorsten, "Comparing 3D Pharmacophore Triplets and 2D Fingerprints for Selecting Diverse Compound Subsets," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, 1999, Vol. 39, No. 6, pp. 1211-1225.

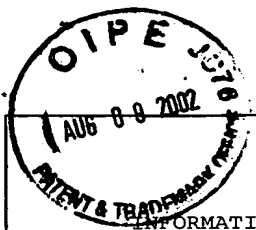
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AB	AN	14	Matter, Hans, "Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-Dimensional and Three-Dimensional Molecular Descriptors," <i>J. Med. Chem.</i> , American Chemical Society, 1997, Vol. 40, No. 8, pp. 1219-1229.
	AO	14	Sadowski, Jens and Kubinyi, Hugo, "A Scoring Scheme for Discriminating between Drugs and Nondrugs," <i>J. Med. Chem.</i> , American Chemical Society, 1998, Vol. 41, No. 18, pp. 3325-3329.
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	AQ	14	Schuffenhauer, Ansgar <i>et al.</i> , "Similarity Searching in Files of Three-Dimensional Chemical Structures: Analysis of the BIOSTER Database Using Two-Dimensional Fingerprints and Molecular Field Descriptors," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, 2000, Vol. 40, No. 2, pp. 295-307.
	AR	14	Turner, David B. <i>et al.</i> , "Rapid Quantification of Molecular Diversity for Selective Database Acquisition," <i>J. Chem. Inf. Sci.</i> , American Chemical Society, 1997, Vol. 37, No. 1, pp. 18-22.

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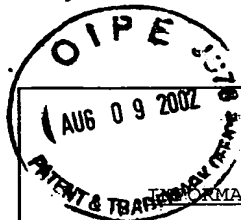
AB	AN	15	Wang, Jing and Ramnarayan, Kal, "Toward Designing Drug-Like Libraries: A Novel Computational Approach for Prediction of Drug Feasibility of Compounds," <i>J. Comb. Chem.</i> , American Chemical Society, November/December 1999, Vol. 1, No. 6, pp. 524-533.
	AO	15	Gasteiger, J. et al, "Assessment of the Diversity of Combinatorial Libraries by an Encoding of Molecular Surface Properties," <i>Abstracts of Papers Part 1: 211th ACS National Meeting</i> , March 24-28, 1996, p. 70-CINF.
	AP	15	Hassan, Moises et al., "Optimization and visualization of molecular diversity of combinatorial libraries," <i>Molecular Diversity</i> , ESCOM Science Publishers B.V., 1996, Vol. 2, pp. 64-74.
	AQ	15	Bellman, R.E., <i>Adaptive Control Processes: A Guided Tour</i> , Princeton Univ. Press, Princeton, NJ (1961).
	AR	15	Bezdek, J.C., <i>Pattern Recognition with Fuzzy Objective Function Algorithms</i> , Plenum Press, New York, NY (1981).

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MB	AN	16	Johnson, M.A., and Maggiora, G.M., <i>Concepts and Applications of Molecular Similarity</i> , John Wiley and Sons, New York, NY (1990).
	AO	16	Kohonen, T., <i>Self-Organizing Maps</i> , Springer-Verlag, Heidelberg, Germany (1995).
	AP	16	Oja, E., <i>Subspace Methods of Pattern Recognition</i> , Research Studies Press, Letchworth, England (1983).
	AQ	16	Agrafiotis, D.K., "A New Method For Analyzing Protein Sequence Relationships Based On Sammon Maps," <i>Protein Science</i> , Cambridge University Press, Vol. 6, No. 2, February 1997, pp. 287-293.
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MB	AN	17	Amzel, L.M., "Structure-based drug design," <i>Current Opinion in Biotechnology</i> , Vol. 9, No. 4, August 1998, pp. 366-369.
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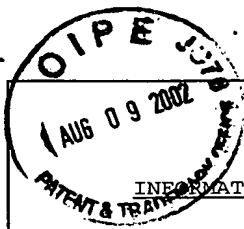
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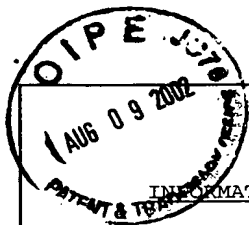
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	AN	18	Eichler, U. et al., "Addressing the problem of molecular diversity," <i>Drugs of the Future</i> , Prous Science, Vol. 24, No. 2, 1999, pp. 177-190.
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	AR	18	Houghten, R.A. et al., "The Use of Synthetic Peptide Combinatorial Libraries for the Identification of Bioactive Peptides," <i>Peptide Research</i> , Vol. 5, No. 6, 1992, pp. 351-358.

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AB	AN	19	Klopman, G., "Artificial Intelligence Approach to Structure-Activity Studies. Computer Automated Structure Evaluation of Biological Activity of Organic Molecules," <i>J. Am. Chem. Soc.</i> , American Chemical Society, Vol. 106, No. 24, November 28, 1984, pp. 7315-7321.
	AO	19	Lajiness, M.S. et al., "Implementing Drug Screening Programs Using Molecular Similarity Methods," <i>QSAR: Quantitative Structure-Activity Relationships in Drug Design</i> , Alan R. Liss, Inc., 1989, pp. 173-176.
	AP	19	Loew, G.H. et al., "Strategies for Indirect Computer-Aided Drug Design," <i>Pharmaceutical Research</i> , Plenum Publishing Corporation, Vol. 10, No. 4, 1993, pp. 475-486.
	AQ	19	Lynch, M.F. et al., "Generic Structure Storage and Retrieval," <i>J. Chem. Inf. Comput. Sci.</i> , American Chemical Society, Vol. 25, No. 3, August 1985, pp. 264-270.
	AR	19	Myers, P.L. et al., "Rapid, Reliable Drug Discovery," <i>Today's Chemist At Work</i> , American Chemical Society, Vol. 6, No. 7, July/August 1997, pp. 46-48, 51 & 53.

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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

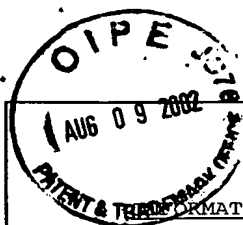
AK	AN	20	Pabo, C.O. and Suchanek, E.G., "Computer-Aided Model-Building Strategies for Protein Design," <i>Biochemistry</i> , American Chemical Society, Vol. 25, No. 20, 1986, pp. 5987-5991.
	AO	20	Saudek, V. et al., "Solution Conformation of Endothelin-1 by H NMR, CD, and Molecular Modeling," <i>International Journal of Peptide Protein Res.</i> , Munksgaard International Publishers Ltd., Vol. 37, No. 3, 1991, pp. 174-179.
	AP	20	Singh, J. et al., "Application of Genetic Algorithms to Combinatorial Synthesis: A Computational Approach to Lead Identification and Lead Optimization," <i>J. Am. Chem. Soc.</i> , American Chemical Society, Vol. 118, No. 5, February 7, 1996, pp. 1669-1676.
	AQ	20	Van Drie, J.H. and Lajiness, M.S., "Approaches to virtual library design," <i>Drug Discovery today</i> , Elsevier Science Ltd., Vol. 3, No. 6, June 1998, pp. 274-283.
	AR	20	Walters, W.P. et al., "Virtual screening - an overview," <i>Drug Discovery today</i> , Elsevier Science Ltd., Vol. 3, No. 4, April 1998, pp. 160-178.

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FORM PTO-1449

## INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO.  
1503.0200006APPLICATION NO.  
09/802,956APPLICANT  
Agrafiotis et al.FILING DATE  
March 12, 2001GROUP  
2123

## U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB- CLASS	FILING DATE
	AA21						
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## FOREIGN PATENT DOCUMENTS

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	AJ21						Yes No
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	AL21						Yes No
	AM21						Yes No

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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	21	Weber, L., "Evolutionary combinatorial chemistry: application of genetic algorithms," <i>Drug Discovery today</i> , Elsevier Science Ltd., Vol. 3, No. 8, August 1998, pp. 379-385.
	AO	21	Weber, L. et al., "Optimization of the Biological Activity of Combinatorial Compound Libraries by a Genetic Algorithm," <i>Angewandte Chemie International Edition in English</i> , VCH, Vol. 34, No. 20, November 3, 1995, pp. 2280-2282.
	AP	21	Graybill, T.L. et al., "Enhancing the Drug Discovery Process by Integration of High-Throughput Chemistry and Structure-Based Drug Design," from <i>Molecular Diversity and Combinatorial Chemistry: Libraries and Drug Discovery</i> , Chaiken and Janda (eds.), American Chemical Society, 1996, pp. 16-27.
	AQ	21	Saund, E., "Dimensionality-Reduction Using Connectionist Networks," <i>IEEE Transactions on Pattern Analysis and Machine Intelligence</i> , IEEE, Vol. 11, No. 3, March 1989, pp. 304-314.
	AR	21	"3DP gains drug research patent", <i>Chemistry in Britain</i> , The Royal Society of Chemistry, Vol. 32, No. 1, January 1996, p. 22.

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Samuel Brooks

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## INFORMATION DISCLOSURE STATEMENT

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	AJ22					Yes No
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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	22	"Accelerate the Discovery Cycle with Chem-XI", Source and date of publication unclear, 2 pages.
	AO	22	Agrafiotis, D. K., "Stochastic Algorithms for Maximizing Molecular Diversity", <i>Journal of Chemical Information and Computer Sciences</i> , American Chemical Society, Vol. 37, No. 5, 1997, pp. 841-851.
	AP	22	Alsberg, B.K. et al., "Classification of pyrolysis mass spectra by fuzzy multivariate rule induction-comparison with regression, K-nearest neighbour, neural and decision-tree methods", <i>Analytica Chimica Acta</i> , Elsevier Science B.V., Vol. 348, No. 1-3, August 20, 1997, pp. 389-407.
	AQ	22	Andrea, T.A. and Kalayeh, H., "Applications of Neural Networks in Quantitative Structure-Activity Relationships of Dihydrofolate Reductase Inhibitors", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 34, No. 9, 1991, pp. 2824-2836.
	AR	22	Aoyama, T. et al., "Neural Networks Applied to Quantitative Structure-Activity Relationship Analysis", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 33, No. 9, 1990, pp. 2583-2590.

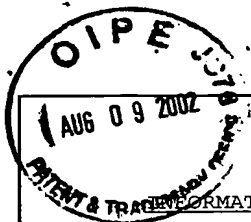
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## PATENT &amp; TRADEMARK INFORMATION DISCLOSURE STATEMENT

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	AJ23						Yes No
	AK23						Yes No
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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	23	Aoyama, T. and Ichikawa, H., "Obtaining the Correlation Indices between Drug Activity and Structural Parameters Using a Neural Network", <i>Chemical &amp; Pharmaceutical Bulletin</i> , Pharmaceutical Society of Japan, Vol. 39, No. 2, February 1991, pp. 372-378.
	AO	23	"ArQule Inc", from <a href="http://www.bioportfolio.com/arqule/products.htm">http://www.bioportfolio.com/arqule/products.htm</a> , 5 pages, (March 18, 1998).
	AP	23	Baum, R.M., "Combinatorial Approaches Provide Fresh Leads for Medicinal Chemistry", <i>Chemical &amp; Engineering News</i> , American Chemical Society, February 7, 1994, pp. 20-26.
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	AR	23	Bottou, L. and Vladimir Vapnik, "Local Learning Algorithms", <i>Neural Computation</i> , Massachusetts Institute of Technology, Vol. 4, No. 6, pp. 888-900, (November 1992).

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Samuel Berda

DATE CONSIDERED

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EXAMINER INITIAL	DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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	AJ24					Yes No
	AK24					Yes No
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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

MB	AN	24	Boulu, L.G. and Crippen, G.M., "Voronoi Binding Site Models: Calculation of Binding Modes and Influence of Drug Binding Data Accuracy", <i>Journal of Computational Chemistry</i> , John Wiley & Sons, Inc., Vol. 10, No. 5, July/August 1989, pp. 673-682.
↓	AO	24	Boulu, L.G. et al., "Voronoi Binding Site Model of a Polycyclic Aromatic Hydrocarbon Binding Protein", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 33, No. 2, 1990, pp. 771-775.
<del>MB</del>	<del>AP</del>	<del>24</del>	<del>Brown, R. D. and Martin, Y.C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection", <i>Journal of Chemical Information and Computer Sciences</i>, Vol. 36, No. 3, 1996, pp. 572-584.</del>
MB	AQ	24	Cacoullos, T., "Estimation of a Multivariate Density", <i>Annals of The Institute of Statistical Mathematics</i> , The Institute of Statistical Mathematics, Vol. 18, No. 2, 1966, pp. 179-189.
↓	AR	24	Clark, R.D., "OptiSim: An Extended Dissimilarity Selection Method for Finding Diverse Representative Subsets", <i>Journal of Chemical Information and Computer Sciences</i> , American Chemical Society, Vol. 37, No. 6, 1997, pp. 1181-1188.

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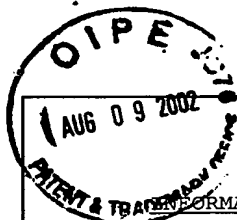
Samuel Booth

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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	25	Clark, D. E., and Westhead, D.R., "Evolutionary algorithms in computer-aided molecular design", <i>Journal of Computer-Aided Molecular Design</i> , ESCOM Science Publishers B.V., Vol. 10, No. 4, August 1996, pp. 337-358.
	AO	25	Cramer, III, R. D. et al., "Comparative Molecular Field Analysis (CoMFA). 1. Effect of Shape on Binding of Steroids to Carrier Proteins", <i>Journal of The American Chemical Society</i> , American Chemical Society, Vol. 110, No. 18, August 31, 1988, pp. 5959-5967.
	AP	25	Cramer, III, R. D. et al., "Substructural Analysis. A Novel Approach to the Problem of Drug Design", <i>Journal of Medicinal Chemistry</i> , Vol. 17, No. 5, May 1974, pp. 533-535.
	AQ	25	Crippen, G. M., "Voronoi Binding Site Models", <i>Journal of Computational Chemistry</i> , John Wiley & Sons, Inc., Vol. 8, No. 7, October/November 1987, pp. 943-955.
	AR	25	Friedman, J. H. et al., "An Algorithm for Finding Best Matches in Logarithmic Expected Time", <i>ACM Transactions on Mathematical Software</i> , Association for Computing Machinery, Vol. 3, No. 3, September 1977, pp. 209-226.

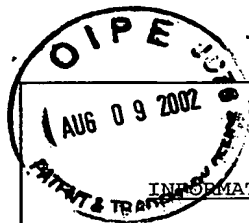
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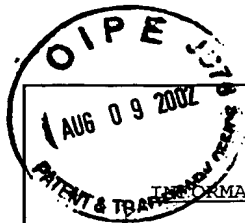
AB	AN	26	Friedman, J.H., "Fitting Functions To Noisy Data In High Dimensions", Department of Statistics- Stanford University Technical Report No. 101, (August, 1988).
	AO	26	Gallop, M. A. et al., "Applications of Combinatorial Technologies to Drug Discovery. 1. Background and Peptide Combinatorial Libraries", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 37, No. 9, April 29, 1994, pp. 1233-1251.
	AP	26	Ghose, A. K. and Crippen, G.M., "Use of Physicochemical Parameters in Distance Geometry and Related Three-Dimensional Quantitative Structure-Activity Relationships: A Demonstration Using <i>Escherichia coli</i> Dihydrofolate Reductase Inhibitors", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 28, No. 3, 1985, pp. 333-346.
	AQ	26	Good, A. C. et al., "Structure-Activity Relationships from Molecular Similarity Matrices", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 36, No. 4, February 19, 1993, pp. 433-438.
	AR	26	Gordon, E. M. et al., "Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic Synthesis, Library Screening Strategies, and Future Directions", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 37, No. 10, May 13, 1994, pp. 1385-1401.

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	AM27					Yes No

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AS	AN	27	Hartigan, J. A., "Representation of Similarity Matrices By Trees", <i>Journal of the American Statistical Association</i> , Vol. 62, No. 320, December, 1967, pp. 1140-1158.
	AO	27	Hopfinger, A. J., "A QSAR Investigation of Dihydrofolate Reductase Inhibition by Baker Triazines Based upon Molecular Shape Analysis", <i>Journal of the American Chemical Society</i> , American Chemical Society, Vol. 102, No. 24, November 19, 1980, pp. 7196-7206.
	AP	27	Jackson, R. C., "Update on computer-aided drug design", <i>Current Opinion in BIOTECHNOLOGY</i> , Current Biology Ltd., Vol. 6, No. 6, December 1995, pp. 646-651.
	AQ	27	Kim, K. H., "Comparative molecular field analysis (CoMFA)", <i>Molecular Similarity in Drug Design</i> , ed. P. M. Dean, Blackie Academic & Professional, 1995, Ch. 12, pp. 291-331.
	AR	27	Kohonen, T., "Self-Organized Formation of Topologically Correct Feature Maps", <i>Biological Cybernetics</i> , Springer-Verlag, Vol. 43, No. 1, 1982, pp. 59-69.

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	AJ28					Yes No
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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	28	Koile, K. and Shapiro, R., "Building A Collaborative Drug Design System", <i>Proceedings of the 25h Hawaii International Conference on System Sciences</i> , IEEE, 1992, pp. 706-716.
	AO	28	Kowalski, B. R. and Bender, C. F., "Pattern Recognition. II. Linear and Nonlinear Methods for Displaying Chemical Data", <i>Journal of the American Chemical Society</i> , American Chemical Society, Vol. 95, No. 3, February 7, 1973, pp. 686-693.
	AP	28	Kruskal, J. B., "Nonmetric Multidimensional Scaling: A Numerical Method", <i>Psychometrika</i> , Vol. 29, No. 2, June, 1964, pp. 115-129.
	AQ	28	Lengauer, T. and Rarey, M., "Computational methods for biomolecular docking", <i>Current Opinion in Structural Biology</i> , Current Biology Ltd, Vol. 6, No. 3, June, 1996, pp. 402-406.
	AR	28	Luke, B. T., "Evolutionary Programming Applied to the Development of Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", <i>Journal of Chemical Information and Computer Sciences</i> , American Chemical Society, Vol. 34, No. 6, November/December 1994, pp. 1279-1287.

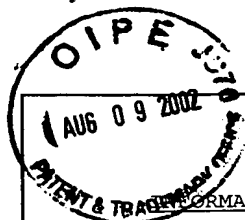
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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

MS	AN	29	Martin, E. J. et al., "Does Combinatorial Chemistry Obviate Computer-Aided Drug Design?", <i>Reviews in Computational Chemistry</i> , VCH Publishers, Inc., Vol. 10, 1997, pp. 75-99.
	AO	29	Martin, E. J. et al., "Measuring Diversity: Experimental Design of Combinatorial Libraries for Drug Discovery", <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 38, No. 9, April 28, 1995, pp. 1431-1436.
	AP	29	McMartin, C. and Bohacek, R.S., "QXP: Powerful, rapid computer algorithms for structure-based drug design", <i>Journal of Computer-Aided Molecular Design</i> , Kluwer Academic Publishers, Vol. 11, No. 4, July 1997, pp. 333-344.
	AQ	29	Mezey, P. G. and Walker, P.D., "Fuzzy molecular fragments in drug research", <i>Drug Discovery today</i> , Vol. 2, No. 4, April 1997, pp. 132-137.
	AR	29	Müller, K., "On the paradigm shift from rational to random design", <i>Journal of Molecular Structure (Theochem)</i> , Elsevier Science B.V., Vol. 398-399, Special Issue, 1997, pp. 467-471.

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Samuel Borda

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	AL30						Yes No
	AM30						Yes No

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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	30	Myers, P., "The Design Of A Universal, Informer™ Library", COMBICHEM, INC., 10 Pages, Date unknown.
	AO	30	Oinuma, H. <i>et al.</i> , "Neural Networks Applied to Structure-Activity Relationships", <i>Journal of Medicinal Chemistry</i> , Vol. 33, No. 3, pp. 905-908, (1990).
	AP	30	Omohundro, S. M., "Bumptrees for Efficient Function, Constraint, and Classification Learning", <i>Advances in Neural Information Processing Systems 3</i> , Morgan Kaufmann, 1991, 7 pages, unknown.
	AQ	30	Parrill, A. L., "Evolutionary and genetic methods in drug design", <i>Drug Discovery today</i> , Elsevier Science Ltd., Vol. 1, No. 12, December 1996, pp. 514-521.
	AR	30	Polanski, J., "A neural network for the simulation of biological systems", <i>Journal of Molecular Structure (Theochem)</i> , Elsevier Science Ltd., Vol. 398-399, Special Issue, 1997, pp. 565-571.

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Samuel Broda

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1503.0200006APPLICATION NO.  
09/802,956APPLICANT  
Agrafiotis et al.FILING DATE  
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EXAMINER INITIAL	DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA31					
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## FOREIGN PATENT DOCUMENTS

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	AJ31					Yes No
	AK31					Yes No
	AL31					Yes No
	AM31					Yes No

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## OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AB	AN	31	Ramos-Nino, M. E. et al., "A comparison of quantitative structure-activity relationships for the effect of benzoic and cinnamic acids on <i>Listeria monocytogenes</i> using multiple linear regression, artificial neural network and fuzzy systems", <i>Journal of Applied Microbiology</i> , Society for Applied Bacteriology, Vol. 82, No. 2, February 1997, pp. 168-176.
	AO	31	Rogers, D. and Hopfinger, A. J., "Application of Genetic Function Approximation to Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", <i>Journal of Chemical Information and Computer Sciences</i> , American Chemical Society, Vol. 34, No. 4, July/August 1994, pp. 854-866.
	AP	31	Sammon, Jr., J. W., "A Nonlinear Mapping for Data Structure Analysis", <i>IEEE Transactions on Computers</i> , IEEE, Vol. C-18, No. 5, May 1969, pp. 401-409.
	AQ	31	Simon, Z. et al., "Mapping of Dihydrofolate-reductase Receptor Site by Correlation with Minimal Topological (Steric) Differences", <i>Journal of Theoretical Biology</i> , Academic Press, Inc., Vol. 66, No. 3, June 7, 1997, pp. 485-495.
	AR	31	Smellie, A. S. et al., "Fast Drug-Receptor Mapping by Site-Directed Distances: A Novel Method of Predicting New Pharmacological Leads", <i>Journal of Chemical Information and Computer Sciences</i> , American Chemical Society, Vol. 31, No.3, August 1991, pp. 386-392.

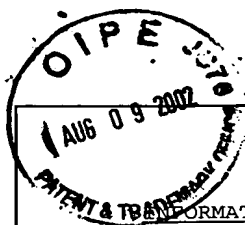
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	AJ32						Yes No
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AB	AN	32	Specht, D. F., "A General Regression Neural Network", <i>IEEE Transactions on Neural Networks</i> , IEEE, Vol. 2, No. 6, November 1991, pp. 568-576.
	AO	32	Svozil, D. et al., "Neural Network Prediction of the Solvatochromic Polarity/Polarizability Parameter $\pi^H_2$ ", <i>Journal of Chemical Information and Computer Sciences</i> , American Chemical Society, Vol. 37, No. 2, 1997, pp. 338-342.
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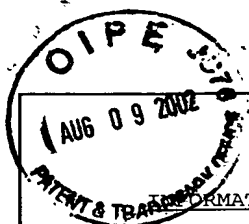
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EXAMINER INITIAL	DOCUMENT NUMBER	DATE	NAME	CLASS	SUB- CLASS	FILING DATE
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## FOREIGN PATENT DOCUMENTS

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	AJ34					Yes No
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	AO	34	Zadeh, L. A., "Communication Fuzzy Algorithms", <i>Information and Control</i> , Academic Press, Vol. 12, No. 2, February 1968, pp. 94-102.
	AP	34	Zadeh, L. A., "Fuzzy Sets", <i>Information and Control</i> , Academic Press, Vol. 8, No. 3, June 1965, pp. 338-353.
	AQ	34	Copy of International Search Report issued April 21, 1998 for Appl. No. PCT/US97/20919, 6 pages.
	AR	34	Copy of International Search Report issued May 13, 1998 for Appl. No. PCT/US97/20918, 7 pages.

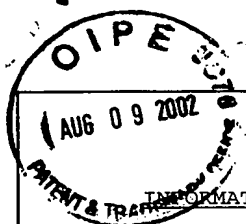
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AB	AN	35	Aoyama, T. et al., "Neural Networks Applied to Structure-Activity Relationships," <i>Journal of Medicinal Chemistry</i> , American Chemical Society, Vol. 33., No. 3, 1990, pp. 905-908.
	AO	35	Gasteiger, J. et al., "Analysis of the Reactivity of Single Bonds in Aliphatic Molecules by Statistical and Pattern Recognition Methods," <i>Journal of Chemical Information Computer Science</i> , American Chemical Society, Vol. 33, No. 3, 1993, pp. 385-394.
	AP	35	Guez, A. and Nevo, I., "Neural networks and fuzzy logic in clinical laboratory computing with application to integrated monitoring," <i>Clinica Chimica Acta</i> , Elsevier Science Publishers B.V., Vol. 248, 1996, pp. 73-90.
	AQ	35	Rouvray, D.H., "Similarity in Chemistry: Past, Present and Future," <i>Topics in Chemistry</i> , Springer-Verlag, Vol. 173, 1995, pp. 1-30.
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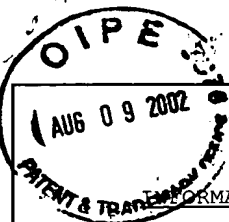
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AB	AN	36	Kim, H. et al., "Self-Organized Distributed Networks for Learning Highly Nonlinear Mapping," <i>Intelligent Engineering Systems Through Artificial Neural Networks</i> , American Society of Mechanical Engineers, Vol. 4, November 13-16, 1994, pp. 109-114.
	AO	36	Pal, N.R. and Eluri, V.K., "Two Efficient Connectionist Schemes for Structure Preserving Dimensionality Reduction," <i>IEEE Transactions on Neural Networks</i> , IEEE, Vol 9, No. 6, November 1998, pp. 1142-1154.
	AP	36	Domine, D. et al., "Non-Linear Mapping for Structure-Activity and Structure-Property Modelling," <i>Journal of Chemometrics</i> , John Wiley & Sons, Ltd., Vol. 7, No. 4, July-August 1993, pp. 227-242.
	AQ	36	Hosenpud, J. et al., "The Effect of Transplant Center Volume on Cardiac Transplant: A Report of the United Network for Organ Sharing Scientific Registry," <i>Journal of the American Medical Association</i> , American Medical Association, Vol. 271, No. 23, June 15, 1994, pp. 1844-1849.
	AR	36	English-language Abstract of European Patent No. 0 355 628, printed from Dialog File No. 351 (February, 1990 - Date of publication of application).

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